GROUNDWATER MODELING GUIDELINES

III. Groundwater Model Design and Application

The purpose of this guideline is to provide direction for the design and application of groundwater models at SRS.

Details

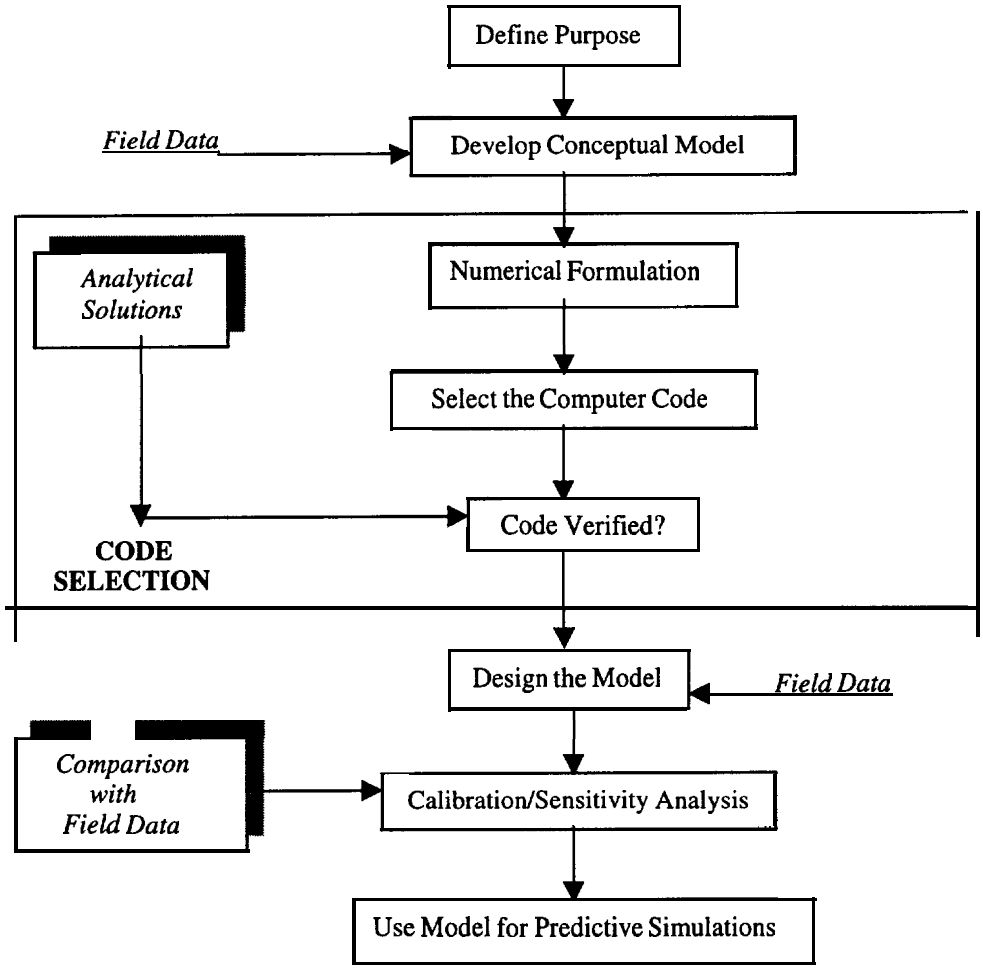
When it has been established that analytical or numerical modeling is necessary and the data are valid, the tasks of model design and application begin. This protocol describes the steps required for analytical and groundwater flow and transport model design and application.

Analytical Modeling

Analytical modeling uses the same general approach as numerical modeling, except for the solution process of the mathematical model. Analytical solutions are used for flow or transport problems as well as aquifer performance tests. In transport problems, analytical solutions may become complex, thus eliminating advantages over numerical methods.

Numerical Modeling

If the complexity of the mathematical model prevents an analytical analysis, numerical models allow for analysis of flow and contaminant transport. The steps required for numerical modeling are summarized in the following diagram. The summation of these steps is creation of a valid, site-specific model that is capable of producing meaningful results.



Steps for Groundwater Flow and Transport Model Design and Application

Step 1
Develop a conceptual model of the system. A conceptual model is a simplified representation of the groundwater flow system, frequently in pictorial form that defines the hydrostratigraphic units of interest and all system boundaries. During this step, field data are assembled including information on water balance and data needed to assign values to aquifer parameters and hydrologic stresses. This includes definition of hydrostratigraphic units and system boundaries.

Step 2
Select the computer code to be used. The code is the computer program that contains an algorithm to numerically solve the mathematical model. Both the governing equation and code should be verified to demonstrate; a) the governing equation accurately describes the physical

processes occurring, and b) the computer program accurately solve the equations that make-up the mathematical model.

Step 3
Design the model. The conceptual model is put into a form suitable for modeling. This step includes grid design, selection of time steps, setting boundary and initial conditions, and preliminary selection of values for aquifer parameters and hydrologic stresses.

Step 4
Calibrate the model. The purpose of calibration is to establish that the model can reproduce field-measured heads and flows within a reasonable margin of error. Calibration is accomplished by trial-and-error adjustment of parameters or by using an automated parameter estimation code.

Step 5
Conduct sensitivity analysis. Sensitivity analysis is performed to ascertain the effects of uncertainty on the calibrated model. The model is influenced by uncertainty owing to the inability to define the exact spatial and temporal distribution of parameter values in the problem domain. There is also uncertainty over definition of boundary conditions and stresses.

Step 6
Use the model for predictive simulations. Prediction quantifies the response of the system to future events. The model is run with calibrated values for parameters and stresses, except for those stresses expected to change in the future. Uncertainty in a predictive simulation arises from uncertainty in the calibrated model and the inability to estimate accurate values for the magnitude and timing of future stresses. Predictive sensitivity analysis quantifies the uncertainty in parameter values on the prediction. Ranges in estimated future stresses are simulated to examine the impact on the model's prediction.

The specific requirements of the above modeling steps are discussed in the following sections.

Step 1 – Develop a Conceptual Model of the System

The reason for constructing a conceptual model is to simplify the field problem and organize the associated field data so that the system can be analyzed more readily. The conceptual model should be as simplified as possible, yet retain enough complexity to adequately reproduce system behavior.

Examples of data used to develop a conceptual model are:

Physical Framework
1. Geologic map and cross sections showing the horizontal and vertical extent and boundaries of the system.
2. Topographic map showing surface water bodies and divides.
3. Contour maps showing the elevation of the base of the aquifers and confining beds.
4. Isopach maps showing the thickness of the aquifers and confining beds.
5. Maps showing the extent and thickness of stream and lake sediments

Hydrogeologic Framework

1. Water table and potentiometric maps for all aquifers.
2. Hydrographs of groundwater head and surface water levels and discharge rates.
3. Maps and cross sections showing the hydraulic conductivity and/or transmissivity distribution.
4. Maps and cross sections showing the storage properties of the aquifers and confining beds.
5. Hydraulic conductivity values and their distribution for streams and lake sediments.
6. Spatial and temporal distributions of rates of evapotranspiration, groundwater recharge, surface water-groundwater interaction, pumping and natural groundwater discharge.

There are three steps in building a conceptual model; A) Define the hydrostratigraphic units and model boundaries, B) Prepare a water budget, and C) Define the flow system.

Substep A – Define the Hydrostratigraphic Units and Model Boundaries

Geologic information such as geologic maps and cross sections, well logs and core descriptions are combined with hydrogeologic data to define hydrostratigraphic units. Hydrostratigraphic units comprise geologic units of similar hydrogeologic properties. These properties may be defined through use of geophysical logs, hydraulic response test data (well injection/extraction tests or slug tests) or via geotechnical evaluations. In some cases, geologic facies can be used to define hydrostratigraphic units. In thick sequences of interbedded sand and clay, model layers may be defined using regional head data to identify units of similar hydrogeologic properties. Site-specific information on stratigraphy and hydraulic conductivity is required to define hydrostratigraphic units on a local scale.

Numerical models require boundary conditions, such that the head or flux must be specified at the borders of the model. Boundary conditions are mathematical statements specifying the dependent variable (flux) at the boundaries of the problem domain. Types of hydrogeologic boundaries are physical boundaries, hydraulic boundaries and hydrogeologic boundaries. Physical boundaries are formed by the presence of an impermeable body of rock or a large body of surface water. Hydraulic boundaries include groundwater divides and streamlines.

The following types of mathematical conditions represent hydrogeologic boundaries:

Type 1. Specified head boundaries (Dirichlet conditions) for which head is given. General Specified Head Boundaries occur wherever head can be specified as a function of position and time over part of the boundary surface of a groundwater system. When the boundary is a river, head along the boundary will vary spatially. For lakes, the boundary is described by constant head conditions.

Type 2. Specified flow boundaries (Neumman conditions) for which the derivative of head (flux) across the boundary is given. Specified flow boundaries describe fluxes to surface water bodies, springflow, underflow and seepage to or from bedrock underlying the modeled system. Specified flow boundaries can also be used to simulate hydraulic boundaries defined from information on the regional flow system.

Type 3. Specifying flux to zero sets no-flow boundary conditions.

Type 4. Head-dependent flow boundaries (mixed-boundary conditions) depend on the difference between the user-supplied specified head on one side of the boundary and the model-calculated head on the other. Examples are leakage to or from a river, lake or reservoir.

Descriptions and examples of the hydrogeologic boundaries are presented in the following table:

Type of Modeled Boundary	Sub-Type of Modeled Boundary	Description	Example
Specified Head, or Dirichlet Boundary Type	General Specified-Head Boundary	Head can be specified as a function of position and time.	Aquifer exposed along the bottom of a stream whose stage is independent of groundwater seepage. Heads along the stream bed are specified according to circumstances external to the groundwater flow system and maintain specified values throughout the problem solution.
Specified Head, or Dirichlet Boundary Type	Constant-Head Boundary	The aquifer system coincides with a surface of unchanging head through time.	Aquifer bordered by a lake where the surface water stage is constant over all points of the boundary in time or position.
Specified Flux, or Neumman Boundary Type	No Flow or Streamline Boundary	The flux across the boundary surface can be specified as a function of position and time (according to circumstances external to the groundwater flow system). The specified flux values are maintained throughout the problem solution.	Impermeable boundary - (if the hydraulic conductivity of adjacent materials differs by orders of magnitude). Groundwater divide – however, may be subject to change with changing conditions and may produce invalid results.
Head Dependent Flux, or Cauchy Type	None	Flux across a part of the boundary surface changes in response to changes in head within the aquifer adjacent to the boundary. A practical limit exists beyond which changes in head cease to cause a change in flux.	The upper surface of an aquifer overlain by a confining bed that is in turn overlain by a body of surface water.
Free-Surface Boundary Type	None	A moveable boundary where the head is equal to the elevation of the boundary (no pressure head).	Water table
Seepage-Face Boundary Type	None	A boundary between the saturated flow field and the atmosphere along which groundwater discharges, either by evaporation or movement "downhill" along the land surface in response to gravity.	Seep line

The steps in boundary definition include:

1. Identification of the physical boundaries of the flow system boundaries - Identify as closely as possible the physical boundaries of the flow system. The 3-D bounding surfaces must be defined (even for 2-D models). Even if the boundaries are far from the area of interest, it is important to understand the location and hydraulic conditions on the flow system boundaries.

2. Formulation of the mathematical representation of the boundaries – Determine the hydraulic condition on the boundaries: specified head, specified flux, head-dependent flux, free surface boundary or seepage face.

3. Examination and sensitivity testing of boundary conditions that change when the system is stressed (stress dependent boundaries) – Test the model to determine the stress dependency of boundaries (to see if natural boundaries are compatible with their representation in the model.) If boundaries are stress dependent, the model cannot be considered a tool for investigating any stress on the system as it will give valid results only when the stresses do not impact the boundary. If not represented correctly, change the boundary type.

4. Revision and final formulation of the initial model boundaries – Based on sensitivity testing (see Step 5 on page 24), revise boundaries and document the stresses for which the boundaries are designed.

Substep B – Prepare a Water Budget

The sources/sinks of the system (recharge/discharge areas) as well as expected flow directions should be included in the conceptual model. The inflows include groundwater recharge from precipitation, overland flow, or recharge from surface water bodies. Outflows may include springflow, baseflow to streams, evapotranspiration and groundwater pumping. The water budget summarizes the magnitudes of inflows and outflows, plus changes in storage. During calibration, this water budget will be used for comparison to the water budget computed by the groundwater model.

Substep C – Define the Flow System

Hydrologic data (precipitation, evaporation and surface water runoff), head data and hydrochemical data are used to conceptualize the movement of groundwater through the system. Water level measurements are used to define the general direction of groundwater flow, the locations of recharge/discharge areas, and the relationships between aquifers and surface water systems. Water chemistry data can be used to define local or regional flow systems, flow direction, sources and amounts of recharge and groundwater flow rates.

Step 2 - Select the Computer Code to be used

The set of commands used to solve a mathematical model forms a computer program, or code. The code solves a set of algebraic equations generated by approximating the partial differential equations (governing equation, boundary conditions and initial conditions) that form the mathematical model. Approximating techniques such as finite difference and finite element methods operate on the mathematical model and change it into a form that can be solved quickly by a computer.

Choosing Finite Difference or Finite Element

The choice between a finite difference and finite element model depends on the problem to be solved and preference of the user. Finite difference methods compute a value for the head at the node (which is also the average head for the cell that surrounds the node). No assumption is made about the form of the variation from one node to the next. Finite elements precisely define the variation in head within an element by means of interpolation (basis) functions. Heads are calculated at nodes for convenience, but head is defined everywhere by basis functions. In

general, fewer input data are needed to construct a finite difference grid, but finite element meshes are better able to approximate irregular boundaries, internal boundaries (such as faults), point sources, sinks, seepage faces and moving water tables.

Groundwater modeling involves simplifying assumptions concerning the parameters being simulated. These parameters will influence the type and complexity of the equations used to represent the model mathematicall y. Five major parameters of groundwater s ystems must be considered when selecting a computer code for simulating groundwater flow, and seven additional parameters for contaminant transport:

Groundwater Flow Parameters

1. Type of Aquifer/Flow Conditions (confined/unconfined, horizontal/vertical, saturated/unsaturated)
2. Matrix Characteristics
3. Homogeneity and Isotropy
4. Fluid Phases
5. Number of Aquifers

Contaminant Transport Parameters

1. Initial Concentration – specify starting concentrations without considering the type of source.
2. Type of Source – point, line, area or volume source.
3. Type of Source Release – release of an instantaneous pulse (or slug) or continuous release.
4. Dispersion – accurate modeling requires incorporation of transport via dispersion.
5. Adsorption – use of a K_d. Non-linear adsorption and temporal/spatial variation are difficult to model.
6. Degradation – easiest when simple first-order degradation coefficients are used. Second-order degradation coefficients (resulting from variations in parameters such as pH, substrate concentration and microbial population) are more difficult. Radioactive decay chains are well known.
7. Density/Viscosity Effects – If the temperature or salinity of the plume differs greatly from ambient conditions, simulations must include the effects of density/viscosity variations.

Typically, the following questions should be answered when selecting a computer code: 1) Has the accuracy of the code been checked (verified) against one or more analytical solutions? 2) Does the code contain a water balance calculation?

Code Verification

The purpose of code verification is to demonstrate that the numerical solution is relatively free of round-off and truncation errors, which can lead to an unstable solution. The comparison of numerical results with an analytical solution will also depend on the choice of error criterion, grid spacing and time step.

In general, the small round-off and truncation errors associated with numerically stable codes are not of concern in solving groundwater problems, except when focusing on the leading edge of contaminant fronts.

Water Balance Calculation

Water balance calculations involves computation of flows across boundaries, to and from sources and sinks and storage. The water balance gives information about discharge rates to surface water bodies, or recharge rates across the water table. Some models provide a node-by-node printout of boundary fluxes, and may compute fluxes between layers. A small error in the water balance is another assurance that the code correctly and accurately solves the mathematical model.

Step 3 - Design the Model

To design the model, it is necessary to specify the model type that bests suits the objectives of modeling, the data set available, the model domain and the conditions encountered at the site. Once the model type has been specified, it is possible to discretize the model domain in time and space. The goal of model design is to simplify the system so it can be analyzed by reasonable means.

The types of available models vary in simplicity, the amount of site-specific data required and the degree of representation of the natural system. Three-dimensional models closely approximate natural conditions, but require extensive site-specific data. Multi-layered models represent stratified aquifers as a combination of 2-D layers linked by leakage. Two-dimensional models neglect flow and transport in either the vertical or horizontal direction, producing predictions in two-dimensions and averaged in the third dimension. If $i^2 << 1.0$ (where i is the gradient), the error in making the two-dimensional assumption for flow is small. The vertical cross section is a 2-D model oriented vertically. Descriptions of models typically used in industry and the modeled processes are presented in the following table:

Name of Model	General Description	Modeled Processes
MODFLOW/ MODFLOWT	2-D or 3-D widely-used, modular, block centered, finite difference model. Additional simulation package handles contaminant transport.	Calculates head distributions, flow rates and water balances. Simulation of advective-dispersive transport with adsorption and first-order decay.
FTWORK	3-D, finite difference, groundwater flow and solute transport model	Advection, hydrodynamic dispersion, adsorption and radioactive decay
MT3D	3-D, finite difference, contaminant transport in groundwater	Advection, dispersion, non-linear sorption, first-order irreversible decay and biodegradation
FACT	3-D finite difference/finite element model used for simulating solute transport in variably and fully saturated media.	Advection, hydrodynamic dispersion, adsorption and first order degradation.

Three-Dimensional Models

Fully 3-D models incorporate all three spatial components of flow in all model cells. The main advantage of 3-D modeling is that simplifying spatial assumptions and heterogeneity are not necessary, and multiple layers, vertical variations and sources can be accommodated with less simplification. Multiple layers, vertical variations and point and area sources can be

accommodated. The disadvantages are the time, expense and data needs for defining and calibrating a 3-D model. Many model cells are used to represent each hydraulic unit, enabling simulation of stratification of flow or transport. Applications that necessitate three-dimensional modeling usually involve:

- Thick aquifers
- Multiple aquifers
- Steeply sloping aquifers
- Multiple or multi-level sinks or sources
- Significant anisotropy or fracturing

Multi-Layered Models

Ideal applications for multi-layered models include sites with many thin aquifers and aquitards that vary in thickness and are not horizontal. A multi-layer model consists of a vertically stacked sequence of 2-D, depth-averaged models that are linked together by sources and sinks. This type of model is quasi 3-D in that horizontal and vertical flow and transport components are simulated. In multi-layered flow models, flow in intervening aquitards is approximated by a leakage term. Flow in aquifer layers is assumed to be horizontal, and flow through aquitards is vertical.

The advantages of the multi-layered approach are that variations in transmissivity of layered aquifers may be simulated by varying thickness of model cells. A complex layered sequence of aquifers or units may be represented by a reasonably small number of model cells. Vertical stratification within aquifers can be simulated by multiple layers.

The disadvantages are:

- Aquifer pinch-outs may not be well simulated
- Steeply sloping aquifers (grade greater than 10%) may not be accurately simulated due to violation of the Dupuit assumption of horizontal flow.

Two-Dimensional Models

Two-dimensional models may be used for four types of aquifers; confined, leaky-confined, unconfined and mixed aquifers.

Discretization of the Model Domain

Selection of the optimum model domain involves balancing the following factors:

- The domain should cover the entire area of interest, including areas that may be effected by future chemical-species transport, and should encompass the effects of internal disturbances (aquifer injection/extraction, or seepage from impoundments). Future transport can be roughly estimated by calculating transport velocities and retardation factors or by analytical solution. The entire chemical-species plume must be included in the model domain, or overall mass balances will not be possible.
- The boundaries of the domain should take advantage of natural groundwater boundaries such as rivers, lakes, drains, groundwater divides, edge of aquifer, boundary between adjacent pumping centers, groundwater recharge/discharge areas, or boundary location distant from the area of interest.
- The model domain should be oriented parallel to the primary groundwater flow direction (in the primary area of interest) to reduce numerical dispersion.

- Available data should be able to adequately define conditions throughout the domain selected.
- Domain size should be minimized to reduce computational effort

Factors that commonly effect model discretization and selection of the model grid include:

Factor	Aspect of Model Discretization Effected
Modeling objectives	Domain size and areas of finer resolution
Area and duration of interest	Domain size
Location of Sources and Sinks	Finer discretization zone
Heterogeneity and anisotropy	Orientation and refinement of grid
Particle velocity and retardation	Cell size and domain size
Natural boundaries	Limit on cell size to simulate boundary
Numerical stability	Limit on ratio of cell sizes
Numerical accuracy	Limit on cell sizes
Computational effort	Limit on total number of cells
Resolution of flow field	Finer discretization where high flow gradient
Resolution of concentration distribution gradient	Finer discretization where high concentration

Selection of time and space dimensionality can be achieved by optimizing the following:
- Enhance model solution stability and convergence.
- Increase model resolution.
- Minimize numerical dispersion.
- Minimize computational requirements for memory, data storage and run time.

Model solution stability and convergence can be improved by the selection of time steps and calculation-mesh cell sizes that are consistent. For example, stability will be ensured by the following condition for a 2-D, transient flow problem (Spitz and Moreno, 1996):

$$0 < dt < \frac{S}{2T} \frac{\Delta x^2 \Delta y^2}{(\Delta x^2 + \Delta y^2)}$$

S = storativity (1/L)
T = transmissivity (L^2/T)
Δx = cell width in the x-dimension (L)
and, Δy = cell width in the y-direction (L)

Accurate predictions require selecting a cell size sufficiently fine to represent local variations in hydraulic head or concentrations, and defining time steps small enough to represent temporal variation of conditions. While variable cell size allows for greater flexibility, highly variable cell sizes can introduce loss in accuracy and stability. Numerical dispersion (or unnatural expansion of a chemical-species plume), occurs due to neglect of higher-order terms in the Taylor Series expansion of the finite difference or finite element formulation of the governing equations. It can

also occur due to inappropriate space or time discretization. Numerical dispersion can be minimized by selection of appropriate mesh cell size, mesh orientation and the size of time steps.

In discretizing a model, the following factors must be considered; 1) the orientation of the model, 2) space discretization, and 3) time discretization.

Orientation of the Model Grid
The following factors must be considered for grid orientation:
- Key hydrologic, hydrogeologic and geologic features of the site – Representation of natural boundaries such as rivers, streams, impoundments, and faults can be simplified by appropriate orientation of the mesh.
- Predominant groundwater flow direction – To minimize numerical dispersion (due to the groundwater velocity being split into components parallel to the calculation mesh axes), orient the mesh along the direction of predominant water flow. If flow direction varies within the model domain, align the mesh with the flow direction in the primary area of interest.
- Anisotropy of hydraulic properties – Since the hydraulic conductivity in the model is expressed as components aligned with the calculation mesh, choose a mesh oriented coincident with the conductivity tensor.

Space Discretization
The resolution of the results provided by the model relates directly to the degree of discretization of the groundwater system. The following factors must be considered in choosing a model grid:
- Degree of heterogeneity in hydraulic transport parameters and boundary conditions
- Model domain size
- The predicted resolution required to meet modeling objectives
- Restrictions imposed by computational resources

These factors also apply to vertical discretization, with the added considerations of stratification due to density effects, recharge, and shallow or deep sources or sinks of groundwater or contaminants. In general, the accuracy of the predicted results improves with finer mesh sizes, but computational time and data space requirements increase correspondingly.

For transport problems, the cell size that minimizes numerical dispersion can be calculated using the Peclet number (Pe), which is the ratio of the advective to diffusive terms in the transport equation. To ensure numerical stability and minimize numerical dispersion, the cell Peclet number should be no greater than 2. The cell Peclet is defined as the dimensionless ratio:

$$Pe = \frac{\Delta x}{\alpha_x} \leq 2$$

Where:

Δx = cell size in the x-direction (L)

and; α_x = longitudinal dispersion in the x-direction (L)

In practice, the Peclet number constraint is often relaxed outside of the area of interest where lower predictive accuracy is acceptable.

The appropriate ratio of the lengths of the cell sides (cell aspect ratio) is calculated by comparing the travel time across the cell in each direction. Ideally, the travel times should be unity, though ratios up to 10:1 may be used without introducing significant error. In general, the greater the variabilit y in cell size, the greater the computational effort required for generating a convergent solution. Cell size increases between adjacent cells no greater than a factor of 1.5 will facilitate model convergence, increase stability and reduce error.

Selection of Time Step

The time step size (Δt) that reduces numerical dispersion can be calculated using the Courant number (Co), which is the ratio of the advective velocity to time-dependent terms in the transport equation:

$$Co = \left| v \frac{\Delta t}{\Delta x} \right| \leq 1$$

To minimize numerical dispersion and maximize stability, the cell Courant number should be no greater than unity for the smallest cell.

Preparing Model Input Data

Field data provide local estimates of conditions, whereas a model requires input of data distributed over the entire model domain. The distribution of data can be accomplished through establishing zones (with homogeneous values within each zone), or by interpolating between data points. For zones, the grid is divided so that sets of nodes have similar aquifer properties based on the extent of the hydrostratigraphic units. The thickness of each unit is assigned to each node.

The head calculation is conducted differently for finite difference and finite element models. A finite difference model calculates the head at the node. In a block-centered-grid, aquifer properties and hydraulic stresses are typically assigned to the block surrounding the node. In a mesh-centered-grid, properties are assigned to the area of influence surrounding the node. In finite element models, aquifer properties may be assigned to the node, element, or area of influence around the node.

Assigning parameter values to the grid requires values for each node, cell or element. Since field data are typically sparse, interpolation of measured data points is necessary for defining the spatial variability over the problem domain. One possible interpolation technique is Kriging, which is a statistical interpolation method that chooses the best linear unbiased estimate for the variable. Higher correlation between measurement points is expected for smaller separation distances. Kriging considers the spatial structure of the variable and provides an estimate of the interpolation error (the standard deviation of the kriged values), while preserving the parameter value at measurement points..

Step 4 - Calibrate the Model

The calibration of a groundwater flow model is the process of adjusting hydraulic parameters, boundary conditions and initial conditions within reasonable ranges to obtain a match between observed and simulated potentials, flow rates, or other calibration targets. The range over which model parameters and boundary conditions may be varied is determined by data presented in the conceptual model. In the case where parameters are well characterized by field measurements, the range over which that parameter is varied in the model should be consistent with the range observed in the field. The degree of fit between model simulations and field measurements can be quantified by statistical means.

Model calibration is frequently accomplished by making trial-and-error adjustments of the model's input data to match field observations. Automatic inverse techniques are another type of calibration procedure. In both trial-and-error and inverse techniques, sensitivity analysis plays a key role in the calibration process by identifying those parameters that are most important in model reliability. Sensitivity analysis is used extensively in inverse techniques to make adjustments to model parameters. The calibration process continues until the degree of correspondence between the simulation and the physical hydrogeological system is consistent with the objectives of the project.

Calibration is evaluated through analysis of residuals. Calibration may be viewed as a regression analysis designed to bring the mean of the residuals close to zero, and to minimize the standard deviation of the residuals. Calibration often necessitates reconstruction of portions of the model, resulting in changes or refinements in the conceptual model to achieve a better representation of the physical system. Calibration to a single set of field measurements does not guarantee a unique solution.

The model calculations may be compared to a second set of field observations that represent a different set of boundary conditions or stresses (a process called model verification). The results are compared to the field measurements to assess the degree of correspondence. If the comparison is not favorable, additional calibration or data collection is required. Successful verification results in a higher degree of confidence in model predictions. A calibrated but unverified model may be used for predictive simulations when coupled with a careful sensitivity analysis. The following steps should be taken for model calibration:

Step 1 - Determine the boundary conditions and model parameters to vary for calibration (ex. hydraulic conductivity, storativity, recharge rates, flow rates, etc.) Also, field measured fluxes such as baseflow, streamflow, infiltration from a losing stream, or evapotranspiration may be selected.

Step 2 - Determine the model calibration targets - measured, observed, calculated or estimated heads or flow rates that a model must reproduce to be considered calibrated (i.e. the calibrated value and its associated error). The error should be a small fraction of the difference between the highest and lowest heads across the site. Errors in the estimates of flow rates are greater than estimates of head.

Step 3 - Determine calibration range over which model parameters and boundary conditions may be varied by data presented in the conceptual model (consistent with the range observed in field measurements).

Step 4 - Decide calibration technique to use (trial-and-error or automatic calibration techniques). In trial and error calibration, after parameter values are initially assigned to each node or element in the grid, they are adjusted in sequential model runs to match simulated heads and flows to calibration targets. The amount of adjustment depends on the range of uncertaint y for each parameter. Automatic calibration (such as automatic inverse modeling) is performed using codes that use either indirect or direct approaches. In a direct solution, the unknown parameters are treated as dependent variables in the governing equation, and heads are independent variables. The indirect approach is similar to trial-and-error in that the forward problem is solved repeatedly (in a systematic way that minimizes the difference between simulated and observed heads or residual statistics).

Step 5 - Perform the calibration When modeling transient conditions, begin with a steady-state scenario to calibrate hydraulic conductivity (or transmissivity). Then, use the transient scenario to calibrate the specific storage (or storativity). Perform the following to make adjustments in the model:

- To raise the hydraulic head at a point in the model, decrease the hydraulic conductivity upstream, increase recharge, decrease the conductance of the boundary nodes to which groundwater at that point discharges, and/or increase flow through the node.
- To speed up the response of water levels at a point to a change in boundary conditions, increase the hydraulic conductivity between that area and the changed boundary, or decrease the specific storage (or storativity) in that area.
- Near a surface water boundary, vary the hydraulic conductivity to raise or lower the slope of the water table (or piezometric surface) and vary the conductance (leakance term) for the boundary or the reference head to raise or lower all water levels nearby by the same amount. If the conductance term is too large, it will function as a constant head boundary.
- To equalize groundwater levels on opposite sides of a confining layer, increase the leakance of the confining layer.
- To remove spatial correlation among residuals, re-parameterize model inputs to define zones of equal parameter values, and smooth transition areas between zones.
- A model with too many constant head boundaries may prove difficult to calibrate. Re-evaluate the conceptual model to determine if boundary conditions are correct.

Step 6 - Analyze calibration qualitatively and quantitatively - Automatic techniques may perform analysis for the modeler. Trial-and-error requires the following analysis:
Qualitatively – assess the distribution of error by comparing contour maps of measured and simulated heads and residuals, and construct scatterplots of data for comparison.
Quantitatively – calculate the differences in measured and simulated head and quantify the average error in the calibration results by calculating the root mean square (RMS) error:

$$RMS = \left[\frac{1}{n} \sum_{i=1}^{n} (h_m - h_s)^2 \right]^{0.5}$$

Where:

h_m = measured heads
h_s = simulated heads
n = the number of observations

The RMS (or standard deviation) is the average of the squared differences in measured and simulated heads.

Step 7 - Repeat the above process until the degree of correspondence between the simulation and the physical hydrogeological system is consistent with the objectives of the project. If the comparison is not favorable, additional calibration or data collection is required.

In summary, the following procedures should be used before and after calibration:

Before Calibration

1. Select calibration values from heads, head gradients, flows or other field data.
2. Estimate the error in the calibration values including measurement error, interpolation error, and errors from scale effects and transient effects. Define calibration targets.
3. Compile the field data needed to set boundary conditions, parameter values, and hydrologic stresses, and estimate plausible ranges in boundary conditions, parameter values and hydrological stresses.
4. Assign parameter values to zones in the grid and calculate the coefficient of variation for each zone.
5. Prepare a map showing the location of calibration targets relative to nodes in the grid.
6. Prepare a table showing initial estimates of boundary conditions, parameters and hydrologic stresses and their coefficients of variation.

After Calibration

1. Calculate coefficients of variation (standard deviation divided by mean value) using calibrated estimates of parameter values. A small coefficient of variation indicates a relatively high degree of certainty. The range of accepted parameter values is determined during calibration and sensitivity analysis.
2. Prepare a table showing differences between calibrated targets and simulated heads and fluxes.

3. Calculate the mean error (ME), mean absolute error (MAE) and RMS error in the heads. The ME is the mean difference between measured heads (h_m) and simulated heads (h_s):

$$ME = \frac{1}{n}\sum_{i=1}^{n}(h_m - h_s)$$

The MAE is the mean of the absolute value of the differences in measured and simulated heads:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left|(h_m - h_s)\right|$$

4. Present the spatial distribution of residual in several ways, selecting from the following types of presentation: (a) map of superimposed contours of head, (b) map showing contours of head residuals, (c) map showing the location and value of calibrated targets and simulated values, (d) plot of calibration values vs. simulated values showing deviation from a straight-line correspondence, (e) box plot of residual heads for each important calibration run, (f) plot of ME, MAE and RMS vs. the calibration run number to show the approach to calibration, (g) plot of ME, MAE, and RMS vs. parameter values to show the sensitivity of the calibration to changes in a parameter value.
5. Prepare a discussion of the calibration procedure and discuss changes in initial parameter estimates and the sensitivity of the model to these changes.

Step 5 - Conduct Sensitivity Analysis

After a groundwater model has been calibrated, sensitivity analysis should be performed. The purpose of sensitivity analysis is to quantify the uncertainty in the calibrated model caused by uncertainty in the estimates of aquifer parameters, stresses and boundary conditions (i.e. identify the model inputs that have the most influence on model calibration and predictions). Sensitivity analysis results in quantitative relationships between model results and the input hydraulic properties or boundary conditions of the aquifer(s). Examination of the sensitivity of calibration residuals and model conclusions to model inputs is a method for assessing the adequacy of the model with respect to its intended function.

Substep A - Identify which model inputs to vary

Identify model inputs that are likely to effect computed head and groundwater flow rates at the times and locations where similar measured quantities exist, and thereby affect calibration results. Calibrated values for hydraulic conductivity, storage parameters, recharge and boundary conditions are systematically changed within the previously established plausible range. Also, identify model inputs that are likely to affect the computed hydraulic heads upon which the models' conclusions are based in the predictive simulations. The magnitude of change in heads from the calibrated solution is a measure of sensitivity of the solution to that particular parameter.

Substep B - Execute calibration and prediction with the value of the input varied over a specific range

For each input: execute calibration and prediction with the value of the input varied over a specific range; graph calibration results and model predictions as functions of the value of input; and determine the type of sensitivity that the model has with respect to the input. Rather than display the effect of every residual, it is appropriate to display residual statistics. The graph should include the following parameters: maximum residual, minimum residual, residual mean, and standard deviation of the residual. In some cases, it may be more illustrative to present contours of head change as a result of variation of input values. In transient simulations, graphs of head change versus time may be presented.

Usually, changing the input value of a single node or element will not significantly affect results. It is important to assemble model inputs into meaningful groups for variation. If the model was not calibrated to multiple hydrologic conditions, variation of more than one type of input at a time can be used to identify potential non-uniqueness of the calibrated input data sets. For each input (or group of inputs) to be varied, the modeler must decide upon the range over which to vary the values. Some should be varied arithmetically, and others geometrically.

Step 6 – Use the Model for Predictive Simulations

In a predictive simulation, the parameters determined during calibration are used to predict the response of the system to future events. The confidence in model predictions is based upon the results of calibration and sensitivity analysis. The two major pitfalls in making predictions are the uncertainty in the calibrated model and uncertainty about future hydrological stresses. In many cases, errors in prediction can be attributed to errors in the conceptual model.

Prediction quantifies the response of the system to future events. The model is run with calibrated values for parameters and stresses, except for those stresses expected to change in the future. Uncertainty in a predictive simulation arises from uncertainty in the calibrated model and the inability to estimate accurate values for the magnitude and timing of future stresses. Predictive sensitivity analysis quantifies the uncertainty in parameter values on the prediction. Ranges in estimated future stresses are simulated to examine the impact on the model's prediction.

The interpretation of the model predictions should include an assessment of where the accuracy of the model is degraded, and the relative degree of uncertainty in the predictions. The uncertainty in the model should be addressed in qualitative and quantitative terms.

The following should be checked to ensure consistency and credibility in model predictions:

- Plot input data and check for accuracy and consistency.
- Check the Courant number for appropriate cell sizes.
- Check the model stability and convergence behavior. Corrections to previous solutions should monotonically decrease with time after each change in stress.
- Check the model flow and solute mass balances.